MATERIAL DATA SHEET

RadonPy PI198, polystyrene family amorphous MD model

Open RadonPy computational screening card for a polystyrene family repeat unit with available amorphous-state physical, thermal, mechanical, dielectric, and optical predictions.

Field	Value
Material ID	radonpy-pi198
Category	Polymer
Condition	amorphous homopolymer computational model | periodic molecular-dynamics cell
Unit system	Common SI
Unit contract	Material properties stored in SI engineering units.
Generated	2026-11-15 23:11

Source and Validity

Field	Value
Quality	Computational screening
Design release allowed	No
Source family	Computational dataset
Confidence	Engineering estimate
License	Open
Source note	BSD-3-Clause RadonPy computed amorphous-polymer record generated from a pinned, hash-checked CSV; no PoLyInfo experimental validation values are included.
Citation	RadonPy PI1070 calculated dataset, commit 840dd4a2b5f261fc9370bb6786eff0b71a463d2f, record PI198, BSD-3-Clause; method DOI 10.1038/s41524-022-00906-4; https://github.com/RadonPy/RadonPy
Valid temperature	300 ... 300 K (Single modeled temperature in the pinned PI1070 CSV.)
Valid pressure	1 ... 1 atm (Upstream pressure input under the LAMMPS real-unit convention.)
Valid phase / condition	RadonPy amorphous homopolymer MD model at 300 K and upstream press=1 (LAMMPS real-unit atmosphere); tacticity=atactic, degree of polymerization=34.
Uncertainty	Classical MD screening result, not a measured grade datasheet. The method paper reports property-dependent bias/correlation limitations; additives, crystallinity, cure, aging, processing, and commercial-grade variation are not represented.
Last reviewed	2026-07-30
Reviewer	scripts/import_radonpy_public_polymers.py
Review status	Checked

Field	Value
Review scope	Checked pinned hashes, BSD attribution, CSV field units, row count, deterministic conversions, and exclusion of PoLyInfo experimental data; not validated for engineering release.
Notes	Computational homopolymer structure, not a supplier grade or formulation.
License ID	BSD-3-Clause
License URL	https://opensource.org/license/bsd-3-clause
Attribution	RadonPy developers; Hayashi et al., npj Computational Materials 8, 222 (2022)

Material Condition

Field	Value
Condition	amorphous homopolymer computational model
Product form	periodic molecular-dynamics cell
Thickness / diameter range	Not applicable to the computational cell.
Test direction	Bulk isotropic modeled response.
Processing route	RadonPy automated all-atom classical molecular-dynamics workflow.
Temperature range	300 ... 300 K
Notes	Classical MD screening result, not a measured grade datasheet. The method paper reports property-dependent bias/correlation limitations; additives, crystallinity, cure, aging, processing, and commercial-grade variation are not represented.

Properties

Physical

Property	Value	Unit	Type	Applies to
Density	1258.2648	kg/m^3	Computed Mean	RadonPy amorphous homopolymer MD model at 300 K and upstream press=1 (LAMMPS real-unit atmosphere); tacticity=atactic, degree of polymerization=34.

Thermal

Property	Value	Unit	Type	Applies to
Specific heat capacity, cp	2579.873926	J/kg/K	Computed Mean	RadonPy amorphous homopolymer MD model at 300 K and upstream press=1 (LAMMPS real-unit atmosphere); tacticity=atactic, degree of polymerization=34.
Specific heat capacity, cv	2461.158063	J/kg/K	Computed Mean	RadonPy amorphous homopolymer MD model at 300 K and upstream press=1 (LAMMPS real-unit atmosphere); tacticity=atactic, degree of polymerization=34.
Volumetric thermal expansion coefficient	0.000550274	1/K	Computed Mean	RadonPy amorphous homopolymer MD model at 300 K and upstream press=1 (LAMMPS real-unit atmosphere); tacticity=atactic, degree of polymerization=34.
Linear thermal expansion coefficient	0.000183425	1/K	Computed Mean	RadonPy amorphous homopolymer MD model at 300 K and upstream press=1 (LAMMPS real-unit atmosphere); tacticity=atactic, degree of polymerization=34.
Thermal conductivity	0.15926394	W/m/K	Computed Mean	RadonPy amorphous homopolymer MD model at 300 K and upstream press=1 (LAMMPS real-unit atmosphere); tacticity=atactic, degree of polymerization=34.
Thermal diffusivity	4.91e-08	m^2/s	Computed Mean	RadonPy amorphous homopolymer MD model at 300 K and upstream press=1 (LAMMPS real-unit atmosphere); tacticity=atactic, degree of polymerization=34.

Mechanical

Property	Value	Unit	Type	Applies to
Bulk modulus	1.653225026	GPa	Computed Mean	RadonPy amorphous homopolymer MD model at 300 K and upstream press=1 (LAMMPS real-unit atmosphere); tacticity=atactic, degree of polymerization=34.
Isentropic bulk modulus	1.726619003	GPa	Computed Mean	RadonPy amorphous homopolymer MD model at 300 K and upstream press=1 (LAMMPS real-unit atmosphere); tacticity=atactic, degree of polymerization=34.

Electrical

Property	Value	Unit	Type	Applies to
Static dielectric constant, dipole-fluctuation term	1.130733691	-	Computed Mean	RadonPy amorphous homopolymer MD model at 300 K and upstream press=1 (LAMMPS real-unit atmosphere); tacticity=atactic, degree of polymerization=34.
Static dielectric constant, electronic-corrected	2.488257122	-	Computed Mean	RadonPy amorphous homopolymer MD model at 300 K and upstream press=1 (LAMMPS real-unit atmosphere); tacticity=atactic, degree of polymerization=34.

Identity

Property	Value	Unit	Type	Applies to
Repeat-unit SMILES	*C(C*)c1c(ccc(c1)Br)OCCCC	-	Model Input	RadonPy amorphous homopolymer MD model at 300 K and upstream press=1 (LAMMPS real-unit atmosphere); tacticity=atactic, degree of polymerization=34.
RadonPy polymer class	2: polystyrene family	-	Computed Classification	RadonPy structural classification of the repeat-unit SMILES.

Model

Property	Value	Unit	Type	Applies to
Number-average molecular mass	8705.34	g/mol	Model Input	RadonPy amorphous homopolymer MD model at 300 K and upstream press=1 (LAMMPS real-unit atmosphere); tacticity=atactic, degree of polymerization=34.
Degree of polymerization	34	-	Model Input	RadonPy amorphous homopolymer MD model at 300 K and upstream press=1 (LAMMPS real-unit atmosphere); tacticity=atactic, degree of polymerization=34.

Optical

Property	Value	Unit	Type	Applies to
Refractive index	1.53541482	-	Computed Mean	RadonPy amorphous homopolymer MD model at 300 K and upstream press=1 (LAMMPS real-unit atmosphere); tacticity=atactic, degree of polymerization=34.

Engineering note: seed solid-material values are reference values only. Verify against the project material specification or supplier data sheet before release.